LLNL-TR-418687

LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Materials and Sensor R&D to Transform the Nuclear Stockpile: Livermore's Transformational Materials Initiative

Robert Maxwell, Larry Fried, Geoff Campbell, Andrew Saab, Jack Kotovsky, Chance Carter, John Chang

October 23, 2009

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Materials and Sensor R&D to Transform the Nuclear Stockpile: Livermore's Transformational Materials Initiative

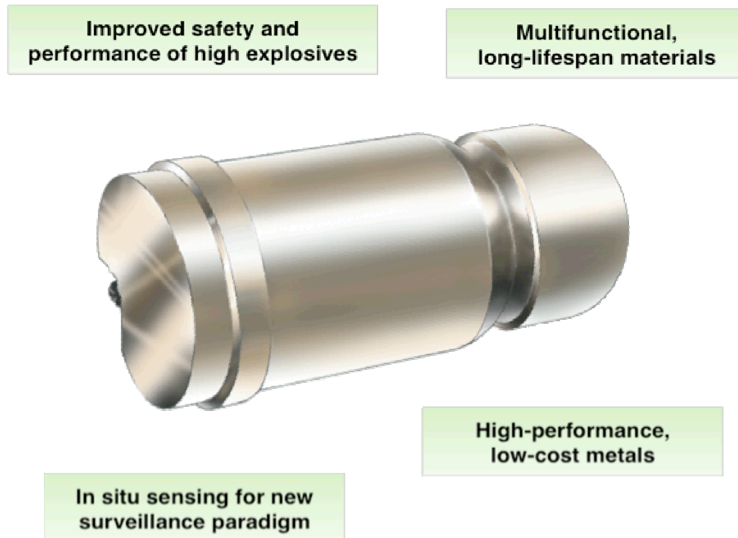
Robert S. Maxwell, Larry Fried, Geoff Campbell, Andrew Saab, Jack Kotovsky, J. Chance Carter, and John Chang

As the nation's nuclear weapons age and the demands placed on them change, significant challenges face the nuclear stockpile. Risks include material supply issues, ever-increasing lifecycle costs, and loss of technical expertise across the weapons complex.

For example, non-nuclear materials are becoming increasingly difficult to replace because manufacturing methods and formulations have evolved in such a way as to render formerly available materials unprofitable, unsafe, or otherwise obsolete. Subtle formulation changes in available materials that occur without the knowledge of the weapons community for proprietary reasons have frequently affected the long-term performance of materials in the nuclear weapon environment. Significant improvements in performance, lifetime, or production cost can be realized with modern synthesis, modeling, and manufacturing methods. For example, there are currently supply and aging issues associated with the insensitive high explosive formulations LX-17 and PBX 9502 that are based on triaminotrinitrobenzene (TATB) and Kel-F, neither of which are commercially available today.

Assuring the reliability of the stockpile through surveillance and regularly scheduled Life Extension Programs is an increasingly expensive endeavor. Transforming our current stockpile surveillance—a system based on destructive testing of increasingly valuable assets—to a system based on embedded sensors has a number of potential advantages that include long-term cost savings, reduced risk associated with asset transportation, state-of-health assessments in the field, and active management of the stockpile.

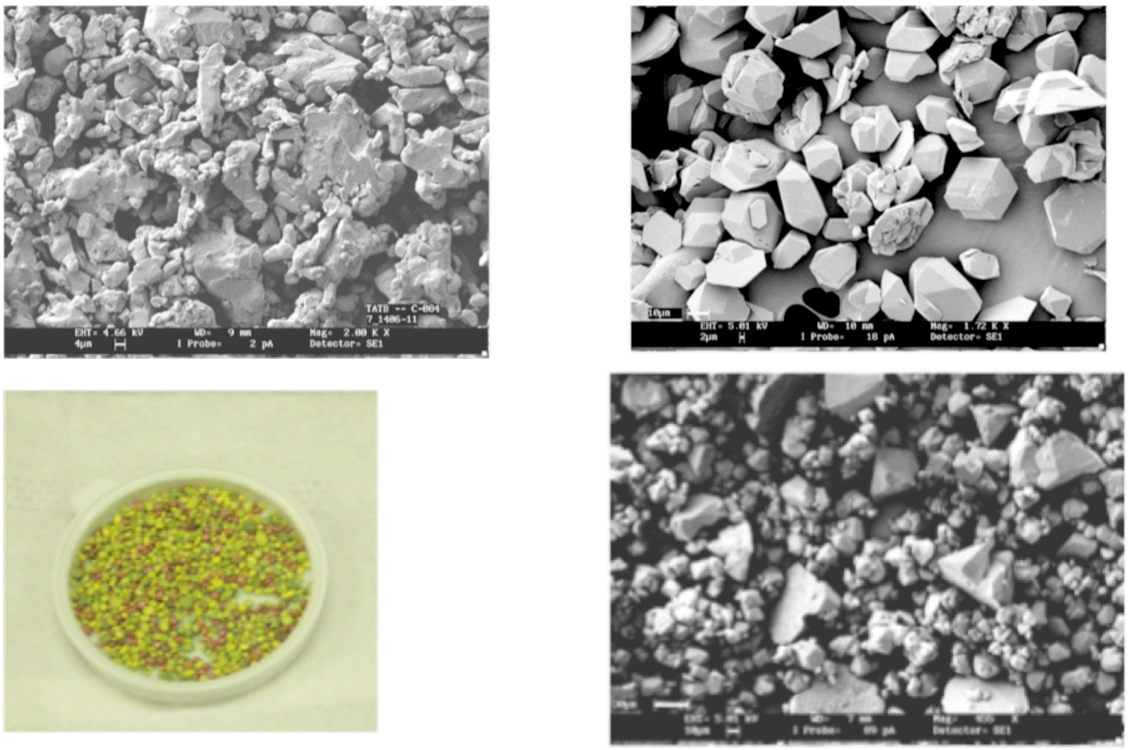
In 2006, Lawrence Livermore National Laboratory initiated the Transformational Materials Initiative (TMI), its largest Laboratory Directed Research and Development (LDRD) project. The TMI united multidisciplinary computational, materials creation and characterization, and sensing expertise to generate valuable intellectual capital for the future needs of the nuclear weapons enterprise, including novel materials and sensing options to improve security of supply, reduced lifecycle costs, and improved lifecycle material and component performance.



A goal of the TMI was to develop materials and approaches that reduce costs and increase reliability of the stockpile.

The TMI focused on a set of thrusts related to the functioning of nuclear weapons: the development and understanding of new insensitive high explosives, new composite metals, new multifunctional polymeric composites, and advanced sensor platforms and materials for weapon applications. Because weapons are integrated designs, TMI integrated these thrusts into a single LDRD Strategic Initiative, which was able to exploit synergies in the multidisciplinary technical teams and streamline management structure. The benefits included delivery of high-quality results with rigorous, integrated project management and external oversight at significantly lower costs than if the overall effort had been executed as individual projects. Though focused on delivering intellectual capital for the future complex, all of the elements of TMI have potential spin-off applications in energy, national security, or conventional weapon applications. The TMI also set out to engage a new generation of materials, sensor, and diagnostic researchers in the core weapons program. This was undertaken with the additional goal of generating high-profile, peer-reviewed publishable research that could also be exploited by new, emerging Laboratory missions. TMI has been spectacularly successful in all these efforts.

Development of New Explosives

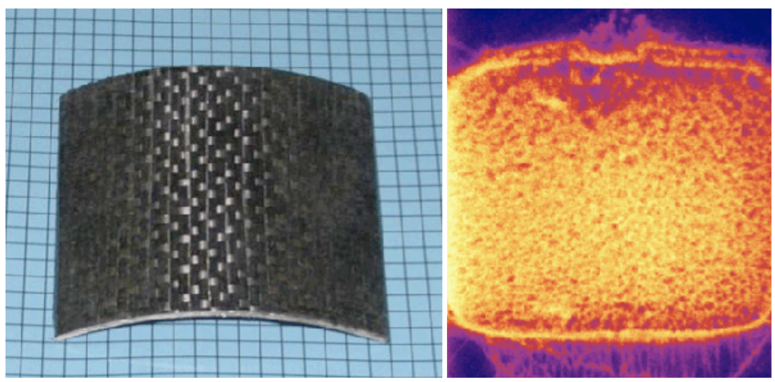


Commercial TATB (top left) and ionic liquid recrystallized TATB from commercial stock (top right). LX-17 molding powder (bottom left) and recrystallized TATB produced from LX-17 molding powder (bottom right).

The TMI specifically generated a new insensitive high-explosive formulation with improved mechanical performance over original materials, yet with nearly identical detonation properties. As part of this effort, the TMI developed a novel approach to recycling and reprocessing dwindling TATB explosive stocks for future use by both the Departments of Energy and Defense. This new approach, based on the use of ionic liquids, enables improvement in particle size control, crystal quality, and morphology, as well as dramatically reducing common impurities. Spin-off work from TMI has also suggested that such ionic liquid reprocessing methods could be of tremendous use in carbon management. The TMI, in fact, demonstrated the ability to produce recrystallized TATB from LX-17 molding powder (a mix of Kel-F and TATB), a process that could be used to replenish TATB stockpiles by recycling LX-17 obtained from weapon dismantlement activities. This has the potential of saving the complex and the country many tens to hundreds of millions of dollars. To improve our understanding of how the recycling process might affect detonation properties, TMI researchers also developed new insights into material detonation.

New Metal Composites

In a second thrust, TMI demonstrated the ability to generate binary composites of metals with improved ductility and lower cost to replace one of the most expensive weapon components. In the process of developing and testing relevant manufacturing and fabrication protocols, modeling and experimental studies led to an improved understanding of the contributions of particle heterogeneities and void structures on high-strain-rate performance of such composites. Of significant benefit, a new low-cost dynamic ductility experiment utilizing conventional high explosives to generate ultrahigh-strain-rate deformation was developed.



Reinforced metal binary composite fabricated by a powder metallurgy process (left). Result of a explosively driven dynamic ductility experiment showing absence of material tearing and fracturing under high-strain-rate deformation (right). This new technique will allow for a significant cost reduction in high-strain-rate screening experiments in the future.

New Polymers

Polymeric organic compounds used as fillers inside nuclear weapons break down over time. TMI researchers generated a number of multifunctional polymeric materials with novel physical or chemical properties and sensing capabilities, while maintaining robust engineering compliance.

These fillers, for example, can sense and absorb hydrogen gas, which can degrade weapon performance. Significant insight into the chemical and physical processes that control the composite formation, structure, functionalized, and ultimate properties was obtained by employing a synergistic combination of multiscale modeling and material characterization studies. The results from these studies helped contribute to an improved understanding of the mechanisms of reinforcement in polymeric nanocomposites.

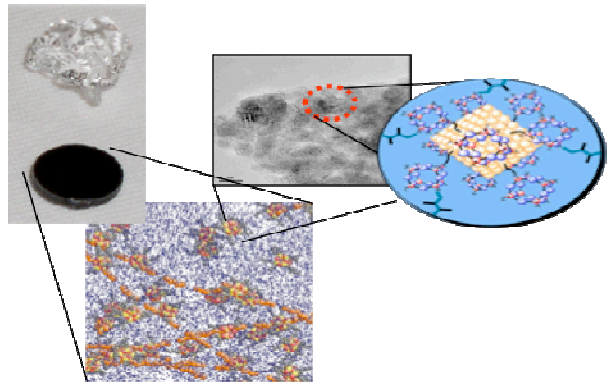


Illustration of a catalytically active silicone composite, with inset electron micrographs of catalytically active palladium nanoparticles with silesquioxane capping agents.

Embedded Sensors

Finally, TMI also successfully developed and demonstrated a number of sensing platforms that show significant promise to transform the surveillance enterprise by continually monitoring weapon health. These tiny embedded sensors will provide instantaneous detection of corrosion, cracks, and composition-changing properties

Stress sensor on top of a dime. Embedded in a nuclear weapon, it can detect changes such as cracks or corrosion in components. Multiple weapon, civilian, and homeland security applications are also possible.

without having to transport and dismantle the weapon. One fiber-based gas sensor detects and captures hydrogen, which is both explosive and corrosive, by using infrared spectroscopy to detect changes in the physical properties of a getter as it captures hydrogen. These sensor platforms have immediate applications both in the weapon programs and in human health and national security applications.

Intellectual Capital

As mentioned earlier, TMI also had the goal of delivering high-quality and high-visibility, peer-reviewed publications and presentations at scientific meetings around the world. Fifty publications have so far resulted from this work, including papers in the prestigious *Science* and *Nature* journals and four cover articles. A number of patents have been granted, have been filed, or are in preparation, and a significant amount of follow-on funding in areas other than defense programs has been obtained. Most significantly, through TMI, a significant number of new scientific and engineering talent has been absorbed by the core weapons programs at Lawrence Livermore, many into key leadership roles.

TMI has produced over 50 publications, including 4 journal cover articles. It has also produced 16 invited and 40 contributed talks, 1 patent, 1 provisional patent, and 16 records of invention.

For further information, contact Robert S. Maxwell [maxwell7@llnl.gov, 925-423-4991].

Publications

1. Armstrong, M. R., et al., *Appl. Phys. Lett*. **92**, 101930 (2008).
2. Baumann, T., et al., *J. Poly. Sci., pt A* (in press).
3. Candy, J. V., et al., *J. Acoust. Soc. Amer.* (in press).
4. Chang, J. T., et al. *IEEE* (submitted).
5. Chang, J. T., et al. *Mag. Comm.* (submitted).

6. Colvin, J. D., et al. *Proceedings of the APS Topical Conference on Shock Compression of Condensed Matter* **955,** 1097 (in press).
7. Crowhurst, J. C., et al., *Science* **319**, 451–453 (2008).
8. Eggimann, Becky L., J. I. Siepmann, and L. E. Fried, *Int. J. Thermophys*. **28**, 796–804 (2007).
9. Fisher, et al., *J. Acoust. Soc. Amer*. **120**(5), 3139 (2006).
10. Fried, L. E., Book Chapter: *Reviews of Computational Chemistry* **25**, 159–184, Wiley-VCH (2007).
11. Gee, R. H., et al., *Macromolecules* **40**, 3422–3428 (2007).
12. Gjersing, E., et al., *Macromolecules* **40**, 4953–4962 (2007).
13. Glascoe, E., et al., *J. Phys. Chem. A* (accepted).
14. Giuliani, J. R., et al., *J. Phys. Chem. B* **111**, 12977–2984 (2007).
15. Goncharov, A. F., et al., *J. Chem. Phys*. **130**, 124514 (2009).
16. Han, T. Y.-J., et al., *New J. Chem*. **10**, 50–56 (2009).
17. Hodge, A. M., et al., *Mater. Sci. Eng. A* **494**, 276–280 (2008).
18. Hoffman, M., et al., *Prop. Exp. Pyro.* (accepted).
19. Jones, et al., *J. Phys. Chem*. (accepted).
20. Kim, S.-S., et al., *Appl. Spectrosc.* **63**, 331–337 (2009).
21. Kim, S.-S., et al., *IEEE Sensor.* (in press).
22. Kim, S.-S., C. Young, and B. Mizaikoff, *Analyt. Bioanalyt. Chem.* **390**, 231–237 (2008).
23. Kotovsky, J., et al., *Sensor. Actuator.* (submitted).
24. Kotovsky, J., et al., *Sensor. Actuator.* (submitted).
25. Lacevic, N., et al., *J. Chem. Phys.* **129**, 124903 (2008).
26. Lacevic, N., L. E. Fried, and R. H. Gee, *J. Chem. Phys.* **128**, 014903 (2008).
27. Letant, S. E., et al., *Cat. Comm*. **8**, 2137–2142 (2007).
28. Lewicki, J. P., et al., *Macromolecules* **41**, 9179–9186 (2008).
29. Maiti, A., et al., *Chem. Phys. Lett.* **440**, 244–248 (2007).
30. Maiti, A., et al., *Chem. Phys. Lett*. (in press).
31. Maiti, A., et al., *J. Appl. Phys*. **103**, 053504 (2008).
32. Maiti, A., et al., *Phys. Chem. Chem. Phys.* **10**, 5050–5056 (2008).

33. Maiti, A., et al., *Poly. Deg. Stab*. **93**, 2226–2229 (2008).
34. Marian, J., J. Knap, and G. H. Campbell *Acta Mater*. **56**, 2389–2399 (2008).
35. Martin, L. P., et al., *Met. Transactions* (accepted).
36. Martin, L. P., A. M. Hodge, and G. H. Campbell, *Scripta Mater*. **57**, 229–232 (2007).
37. Maxwell, R. S., et al., Book Chapter: *Polymer Durability and Radiation Effects*, ACS Symposium series **978**, 1–15 (2008).
38. Mayer, B. P., et al. *Chem. Eng. Sci.* (in press).
39. Mayer, B. P., J. A. Reimer, and R. S. Maxwell, *Macromolecules* **41**, 1323–1327 (2008).
40. Mundy, C. J., et al., *J. Chem. Phys.* **128**, 184701 (2008).
41. Orme, C.A., Book Chapter: *Perspectives on Inorganic, Organic, and Biological Crystal Growth*, vol. 916, p. 342 (2007).
42. Patel, M., et al., *Poly. Deg. Stab*. **93**, 513–519 (2008).
43. Pearman, W. F., et al., *Appl. Optic.* **47**, 4627–4632 (2008).
44. Pearman, W. F., et al., *Appl. Spectrosc*. **62**, 285–289 (2008).
45. Rai, N., et al., *J. Chem. Phys.* **129**, 194510 (2008).
46. Reed, E. J., et al., *Nat. Phys.* **4**, 72–76 (2008).
47. Sirbuly, D. J., et al. *Adv. Mater.* **20**, 4724–4727 (2008).
48. Weisgraber, T. H., et al., *Polymer* (accepted).
49. Wiley, T., et al., *Prop. Exp. Pyro*. (accepted).
50. Wu, C. J., et al., *Nat. Chem.* **1**, 57–62 (2009).